Carfentrazone-ethyl 128639-02-1 | DTXSID4032532

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Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 9.28

Global applicability domain: Inside

Local applicability domain index: 9.74e-01

Confidence level: 5.16e-01

Nearest Neighbors from the Training Set

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2,2',3,4,4',5'-Hexachlorobiphenyl

Measured: 9.80 Predicted: 9.29

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2,2',4,4',5,5'-Hexachlorobiphenyl

Measured: 9.73 Predicted: 9.70

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2,2',3,4',5',6-Hexachlorobiphenyl

Measured: 9.27 Predicted: 9.70

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(+/-)-Oxychlordane Measured: 8.39 Predicted: 9.71

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2,2',4,4',6,6'-Hexachlorobiphenyl

Measured: 8.99 Predicted: 9.93